

Lecture 2: Quantum geometry in moire materials and non-equilibrium flat band transport

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Winter theory school: New Frontiers in Superconductivity, Florida 2024

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- Basics of quantum geometry
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Twisted Bilayer Graphene (TBG) superconductivity since 2018

Reviews: Balents, Dean, Efetov, Young, Nat Phys 2020 Andrei, Efetov, Jarillo-Herrero, MacDonald, Mak, Senthil, Tutuc, Yazdani, Young, Nat Rev Mater 2021



Figure credits see Fig.1 in PT, Peotta, Bernevig, Nat Rev Phys 2022

Geometric contribution in TBG superconductivity





Aleksi Julku

Teemu Peltonen

Long Liang

Tero Heikkilä

Julku, Peltonen, Liang, Heikkilä, PT, PRB(R) (2020); Editors' Suggestion



MA-TBG: Magic Angle-Twisted Bilayer Graphene Twisting graphene layers produces flat bands (unconventional) superconductivity



Y Cao et al. Nature 556, 43–50 (2018)

Also Nature 556, 80 (2018) Science 363, 1059 (2019) Nature 574, 653-657 (2019))

VIEWPOINT



Geometry Rescues Superconductivity in Twisted Graphene

Laura Classen

School of Physics and Astronomy, University of Minnesota, Minneapolis, MN, USA

February 24, 2020 • Physics 13, 23

Three papers connect the superconducting transition temperature of a graphene-based material to the geometry of its electronic wave functions.



APS/Alan Stonebrake

Figure 1: Electrons moving through the sheets of twisted bilayer graphene (TBG) have special points in their band structure where two cone-shaped bands meet. The inherent "curvature" of the states in these bands turns out to contribute to the magnitude of TBG'... Show more

On its own, a sheet of graphene is a semimetal—its electrons interact only weakly with each other. But as experimentalists discovered in 2018 [1, 2], the situation changes when two sheets of graphene are stacked together, with a slight ($\sim 1^{\circ}$) rotation between them (Fig. 1). At this so-called magic twist angle [3] and at low temperatures [1], the electrons become correlated, forming insulating or superconducting phases depending on the carrier density [2–7]. These phases appear to come from a twist-induced flattening of the electronic energy bands, which

Geometric and Conventional Contribution to the Superfluid Weight in Twisted Bilayer Graphene

Xiang Hu, Timo Hyart, Dmitry I. Pikulin, and Enrico Rossi

Phys. Rev. Lett. 123, 237002 (2019)

Published December 5, 2019

Read PDF



Topology-Bounded Superfluid Weight in Twisted Bilayer Graphene

Fang Xie, Zhida Song, Biao Lian, and B. Andrei Bernevig

Phys. Rev. Lett. 124, 167002 (2020)

Published April 24, 2020

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Non-interacting bands



Non-interacting bands



At magic angle $\theta \sim 1$ deg, the number of lattice sites per unit cell (LS) around 13 000: numerically still a problem even at the mean-field level

We reduce LS to around 700 by applying a rescaling trick which modifies the twist angle but keeps the Moire periodicity and the Dirac velocity invariant Fermi-Hubbard lattice model with TBG geometry (600 bands)

$$H = \sum_{ij\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + H_{\rm int}$$

Two pairing schemes

Non-local (RVB) interaction

Local (s-wave) interaction



$$H_{\rm int} = \frac{J}{2} \sum_{\langle ij \rangle} h_{ij}^{\dagger} h_{ij}$$

 $h_{ij} = c_{i\downarrow}c_{j\uparrow} - c_{i\uparrow}c_{j\downarrow}$



$$H_{\rm int} = J \sum_{i} c^{\dagger}_{i\uparrow} c_{i\uparrow} c^{\dagger}_{i\downarrow} c_{i\downarrow}$$

J< 0 is attractive interaction strength

BKT temperature



For flat band regime local interaction has considerably larger T_{BKT}

Here RVB (resonance valence bond) is the non-local pairing scheme



Nematic order parameter for non-local pairing

Local pairing preserves the lattice symmetries and yields isotropic D^s

Non-local pairing breaks the rotational symmetry and yields non-isotropic response

Local pairing has s wave symmetry, non-local yields mixed s+p+d symmetry (d dominant)

$$D^{s} = \begin{bmatrix} D_{xx}^{s} & D_{xy}^{s} \approx 0\\ D_{yx}^{s} \approx 0 & D_{yy}^{s}, \end{bmatrix}$$





Euler class bound of TBG superconductivity: Xie, Song, Lian, Bernevig, PRL (2020)

TBG theory has advanced since 2020 (e.g. Kang, Vafek, PRB 2023; Vafek, Kang, PRB 2023); quantitative predictions to be revisited

First experiments exploring quantum geometric superconductivity in TBG

Tian, Gao, Che, Xu, Cheung, Watanabe, Taniguchi, Randeria, Zhang, Lau, Bockrath, Nature 2023

$$\begin{split} \xi &= \sqrt{\frac{\Phi_0}{2\pi B_{c2}}} \quad \Phi_0 = \frac{h}{2e} \quad J_{cs} = n_s e \frac{\Delta}{\hbar k_F} \\ \text{Critical field and current measured} \\ \text{as well as Fermi velocity} \\ \text{Superfluid weight from} \\ D_s(0) &= \frac{2\pi J_{cs}\xi}{\Phi_0} \\ \text{Isolated flat band} \\ [D_s]_{ij} &= \frac{2}{\pi \hbar^2} \frac{\Delta^2}{UN_{\text{orb}}} \mathcal{M}_{ij}^{\text{R}} \\ \end{split}$$

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New phenomena also in the flat band normal state

In certain lattice models, only pairs move at any temperature, Tovmasyan, Peotta, Liang, PT, Huber, PRB 2018



Aharonov-Bohm effect in a ring geometry

Non-Fermi liquid features in double occupancy and entropy (Lieb lattice), Kumar, Peotta, Takasu, Takahashi, PT, PRB(L) 2021

Insulator – pseudogap crossover in the Lieb lattice normal state, Huhtinen, PT, PRB(L) (2021)

Preformed pairs in a flat band

Tovmasyan, Peotta, Liang, PT, Huber, PRB 2018

What are the charge carriers in the *normal state* of a flat band superconductor? We find: only pairs move (Pi-periodic ground state); non Landau-Fermi liquid.



Related to local conserved quantities.

Flat band interacting normal state; Lieb lattice

- Non-Fermi liquid features in double occupancy and entropy
- SU(N) scaling relation









Pramod Kumar Sebastiano Peotta Yosuke Takasu Yoshiro Takahashi P Kumar, S Peotta, Y Takasu, Y Takahashi, PT, PRB(L) 2021

Lieb lattice: repulsive Hubbard model

Normal state properties

average double occupancy (DMFT)





half-filling: flat band significant

Non-Fermi liquid behavior for small interactions at the flat band

lowest band filled

Insulator – pseudogap crossover in the Lieb lattice normal state



Kukka-Emilia Huhtinen

KE Huhtinen, PT, PRB(L) (2021)

$$\Sigma(\mathbf{k}) \approx \Sigma_{\text{loc}}$$

$$\mathcal{G}(\mathbf{k}) = \left[(\mathcal{G}^0(\mathbf{k}))^{-1} - \Sigma(\mathbf{k}) \right]^{-1}$$

$$\mathcal{G}_{\rm loc} = \left[(\mathcal{G}_{\rm loc}^0)^{-1} - \Sigma_{\rm loc} \right]^{-1}$$

Hubbard model on the Lieb lattice

FOCUS ON THE NORMAL STATE ABOVE SUPERCONDUCTIVITY



Attractive Hubbard model

$$H = \sum_{\sigma} \sum_{i\alpha,j\beta} t_{ij} c^{\dagger}_{\sigma,i\alpha} c_{\sigma,j\beta} - \sum_{\sigma} \sum_{i\alpha} \mu_{\sigma} n_{\sigma,i\alpha} + U \sum_{i\alpha} (n_{\uparrow,i\alpha} - 1/2) (n_{\downarrow,i\alpha} - 1/2)$$

Flat band states reside at $\,A\,{\rm and}\,C\,$ sites

DMFT cluster: A, B and C

DMFT

Georges, Kotliar, Krauth, Rozenberg, Rev. Mod. Phys. 1996 Kotliar, Savrasov, Haule, Oudovenko, Parcollet, Marianetti, Rev. Mod. Phys. 2006

Dynamical Mean Field Theory (DMFT) to capture quantum effects beyond mean-field



Single site DMFT

Cellular/cluster DMFT; Non-local correlations

Large (U>t) interactions: pseudogap



Generalized spin susceptibility: $\chi_{\alpha\alpha}^{\rm spin} = \frac{2}{\beta^2} \sum_{\omega,\omega'} \left(\chi_{\uparrow\alpha,\uparrow\alpha,\uparrow\alpha,\uparrow\alpha}^{\rm ph,\omega,\omega',\nu=0} - \chi_{\uparrow\alpha,\uparrow\alpha,\downarrow\alpha,\downarrow\alpha}^{\rm ph,\omega,\omega',\nu=0} \right) \xrightarrow{\mathbf{+}} \underbrace{\mathbf{+}}_{\mathbf{-}} \underbrace{\mathbf{+}}_{\mathbf{-}} \underbrace{\mathbf{+}}_{\mathbf{-}} \underbrace{\mathbf{+}}_{\mathbf{-}} \underbrace{\mathbf{-}}_{\mathbf{-}} \underbrace{\mathbf{-}} \underbrace{\mathbf{-}}$



Local contribution to spin susceptibility decreases sharply with temperature at $A/C\,$ sites.

At low temperatures, $\beta G_{\alpha\alpha}(\beta/2) \approx \mathcal{A}_{\alpha}(\omega = 0)$, where \mathcal{A}_{α} is the orbital-resolved spectral function.

As interaction is increased, the spectral function becomes depleted around half-filling.

Low interaction (U<t): insulator



$$Z = \left(1 - \frac{\mathrm{Im}\Sigma(i\omega_n)}{\omega_n}\Big|_{\omega_n \to 0}\right)^{-1}$$

In DMFT, $Z = m/m^*$, where m is the bare mass and m^* is the effective mass.

The self-energy diverges at low frequencies when the interaction strength is decreased.

The temperature dependence is $T^{-1/2}\,$ rather than $T^{-1}\,$ found for Mott insulator.

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SYNOPSIS



Static Electrons in Flat-Band Nonequilibrium Superconductors

May 25, 2023 • Physics 16, s76

Single electrons stay stationary in superconductors with "flat-band" electronic structures, which could lead to low-energy-consumption devices made from such materials.

Suppression of Nonequilibrium Quasiparticle Transport in Flat-Band Superconductors

Ville A. J. Pyykkönen, Sebastiano Peotta, and Päivi Törmä

Phys. Rev. Lett. 130, 216003 (2023) Published May 25, 2023





Ville Pyykkönen

Sebastiano Peotta

Flat, edge and dispersive states in the sawtooth ladder



Flat band transport in Keldysh formalism



Hartree potential

$$V_{H,\alpha i}(t) = U_{\alpha i} \langle \hat{c}^{\dagger}_{\alpha i\uparrow}(t) \hat{c}_{\alpha i\uparrow}(t) \rangle$$

Keldysh formalism, non-equilibrium Green's functions

Dyson equation
$$G^{R/A}(\omega) = g^{R/A}(\omega) + g^{R/A}(\omega)\Sigma^{R/A}(\omega)G^{R/A}(\omega)$$

Kadanoff-Baym kinetic equation

$$G^{<}(\omega) = \left[I + G^{R}(\omega)\Sigma^{R}(\omega)\right]g^{<}(\omega)\left[I + \Sigma^{A}(\omega)G^{A}(\omega)\right] + G^{R}(\omega)\Sigma^{<}(\omega)G^{A}(\omega)$$

Transport



Superconducting junction: at finite interaction flat band AC Josephson current is finite but DC current (multiple Andreev reflections) quenched

Normal-normal and normal-superconducting junction: flat band current is quenched

Quasiparticle transport quenched at flat band! Pure supercurrent!

Quasiparticle transport quenched at flat band! Pure supercurrent!

Quasiparticle poisoning

Nonequilibrium Quasiparticles and 2e Periodicity in Single-Cooper-Pair Transistors

J. Aumentado, Mark W. Keller, John M. Martinis, and M. H. Devoret Phys. Rev. Lett. **92**, 066802 – Published 13 February 2004





Four transmons. FJ.M. Gambetta, J.M. Chow, and M. Steffen (npj QuantumInformation 3:2, 2017) by CC BY 4.0 license

G. Catelani and J. P. Pekola, Using materials for quasiparticle engineering, Materials for Quantum Technology 2, 013001 (2022)

D. Rainis and D. Loss, Majorana qubit decoherence by quasiparticle poisoning, Phys. Rev. B 85, 174533 (2012)

Majorana nanowire. H. Zhang, D.E. Liu, M. Wimmer, L.P. Kouwenhoven (Nat Commun 10, 5128, 2019) by CC BY 4.0 license

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Conductivity in a flat band



Kukka-Emilia Huhtinen

KE Huhtinen, PT, PRB (2023)

Conductivity in a flat band

Semiclassical Boltzmann theory of transport:

$$\sigma_{\mu\nu}(\omega) = -\frac{e^2}{\hbar} \sum_n \int_{\text{B.z.}} \frac{d^D \mathbf{k}}{(2\pi)^D} \frac{\partial n_F(E)}{\partial E} \Big|_{E=\epsilon_n(\mathbf{k})} \partial_\mu \epsilon_n(\mathbf{k}) \partial_\nu \epsilon_n(\mathbf{k}) \frac{\eta}{(\hbar\omega)^2 + \eta^2} \qquad \partial_\mu = \partial/\partial k_\mu$$

Full Kubo-Greenwood formula:

$$\sigma_{\mu\nu}(\omega) = \frac{e^2}{i\hbar V} \sum_{\mathbf{k}} \sum_{mn} \frac{n_F(\epsilon_n(\mathbf{k})) - n_F(\epsilon_m(\mathbf{k}))}{\epsilon_n(\mathbf{k}) - \epsilon_m(\mathbf{k})} \frac{[j_\mu(\mathbf{k})]_{nm}[j_\nu(\mathbf{k})]_{mn}}{\epsilon_n(\mathbf{k}) - \epsilon_m(\mathbf{k}) + \hbar\omega + i\eta}$$
$$[j_\mu(\mathbf{k})]_{mn} = \partial_\mu \epsilon_m(\mathbf{k}) \delta_{mn} + (\epsilon_m(\mathbf{k}) - \epsilon_n(\mathbf{k})) \langle \partial_\mu m_\mathbf{k} | n_\mathbf{k} \rangle$$

At low temperatures and finite scattering rate η , the interband geometric part is dominant on a flat band.

Insprired by

- G. Bouzerar and D. Mayou, Phys. Rev. B 103, 075415 (2021)
- J. Mitscherling and T. Holder, Phys. Rev. B 105, 08515 (2022)
- B. Mera and J. Mitscherling, Phys. Rev. B 106, 165133 (2022)
- G. Bouzerar, Phys. Rev. B 106, 125125 (2022)

Conductivity in a flat band

Streda formula:

$$\sigma_{\mu\nu}^{\rm sym}(\omega=0) = -\frac{e^2}{\hbar\pi} \int_{-\infty}^{\infty} \mathrm{d}\epsilon \frac{\partial n_F(\epsilon)}{\partial \epsilon} \operatorname{Tr}[\operatorname{Im}[G_{\boldsymbol{k}}(\epsilon+i\eta)]j_{\mu}(\boldsymbol{k})\operatorname{Im}[G_{\boldsymbol{k}}(\epsilon+i\eta)]j_{\nu}(\boldsymbol{k})] G_{\boldsymbol{k}}(E) = (E-H_{\boldsymbol{k}})^{-1}$$

This gives a result proportional to the integrated quantum metric in the limit $\eta \to 0^+$ when $T \to 0$ is taken *first*.

This occurs only in *perfectly* (partially) flat bands due to ill-defined terms for states at the Fermi energy. The Kubo-Greenwood and Streda formulas do not give the same conductivity when a flat band is in the vicinity of the Fermi energy.



Lack of Fermi surface requires extra care in transport calculations.

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Drude weight and the many-body quantum metric





Grazia Salerno

Tomoki Ozawa

Salerno, Ozawa, PT, PRB Letter (2023)

The many-body quantum metric (MBQM)

Defined on many-body states with respect to the twisted boundary condition phase

$$\mathfrak{g}(\phi) = \operatorname{Re}\left[\left\langle \partial_{\phi} \Psi_0 \right| \left(1 - \left| \Psi_0 \right\rangle \left\langle \Psi_0 \right| \right) \left| \partial_{\phi} \Psi_0 \right\rangle \right]$$

determines the "quantum distance" along a given path in ϕ space.

Many-body generalization of the quantum metric

$$\mathfrak{g}(0) = \operatorname{Re}\left[\sum_{m \neq 0} \frac{|\langle \Psi_m | \partial_{\phi} \hat{H}(\phi) | \Psi_0 \rangle|^2}{(E_m(0) - E_0(0))^2}\right]$$

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$$\partial_{\phi}\hat{H}(\phi) = L\partial_{\Phi}\hat{H}(\Phi) = \hat{J} + \mathcal{O}(\Phi)$$

Drude weight and twisted boundary conditions



Superfluid response of the system to a small external flux Φ introduced by the twisted boundary conditions:

$$D_w = \pi L \left. \frac{\partial^2 E(\Phi)}{\partial \Phi^2} \right|_{\Phi=0}$$

$$\hat{H}(\Phi) = \hat{K}e^{i\Phi/L} + \hat{K}^{\dagger}e^{-i\Phi/L} + \hat{H}_V + \hat{H}_U$$

Drude weight within perturbation theory

 $\mathbf{\alpha}$

Can be bounded by the many-body quantum metric if the system has a gap ϵ

Independent of particle statistics and spatial dimensions!

Summary

Quantum geometry is relevant for any transport or interaction phenomena where overlaps and localization properties of Wannier functions are important – a new viewpoint to condensed matter physics: not only the band structure, but the structure of the Bloch functions



Outlook

Superconductivity at elevated temperatures







Institute



